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=> d his

     (FILE 'HOME' ENTERED AT 10:35:52 ON 29 NOV 2006)
     FILE 'CA' ENTERED AT 10:36:01 ON 29 NOV 2006
L1   1998 S (PH OR ACID? OR BASE OR DEPROTONA?)(3A)(DEPEND? OR VARIAB? OR
          VARY? OR INSTABIL? OR SENSITIV?)(8A)FLUORESC?
L2     23 S L1 AND (LABIL?(2A)(HYDROGEN OR H OR PROTON) OR METHYLAT? OR
          ETHYLAT? OR ALKYLA?)

=> d bib,ab l2 1-23

L2   ANSWER 8 OF 23  CA  COPYRIGHT 2006 ACS on STN
AN   129:181947  CA
TI   UV/Vis and fluorescence study on anthralin and its alkylated derivatives
AU   Sellmer, Andreas; Terpetschnig, Ewald; Wiegrebe, Wolfgang; Wolfbeis,
     Otto S.
CS   Dep. Pharm. Chem. I, Univ. Regensburg, Regensburg, D-93040, Germany
SO   Journal of Photochemistry and Photobiology, A: Chemistry (1998), 116(1),
     39-45
AB   Anthralin and some of its C-10 or O-alkylated derivs. were investigated
     by UV/VIS- and fluorescence spectroscopy in different solvents and
     buffer systems, resp.  The effects of substituents on the formation of
     anthralin anion as well as the constitution of the resulting anions
     confirm that C-H acidity at position 10 is necessary for the formation
     of a fully arom. anionic form.  It is concluded that the resulting anion
     is the pharmacol. active species of the antipsoriatic anthralin.
     Tautomerism of the neutral mol. is not observable.

L2   ANSWER 14 OF 23  CA  COPYRIGHT 2006 ACS on STN
AN   118:191020  CA
TI   Fluorescent species of 7-azaindole and 7-azatryptophan in water
AU   Chen, Y.; Rich, R. L.; Gai, F.; Petrich, J. W.
CS   Dep. Chem., Iowa State Univ., Ames, IA, 50011, USA
SO   Journal of Physical Chemistry (1993), 97(9), 1770-80
AB   A study of the fluorescence lifetimes and quantum yields of 7-azaindole
     and its methylated derivs. N1-methyl-7-azaindole (1M7AI) and 7-methyl-
     7H-pyrrolo[2,3-b]pyridine (7M7AI) in water is performed in order to
     explain the observation that the fluorescence spectrum of 7-azaindole
     apparently consists of one band (λmax = 386 nm) whereas in alcs. the
     spectrum is bimodal (e.g., for methanol, λmax = 374, 505 nm).  Careful
     measurements of the fluorescence decay as a function of emission
     wavelength indicate a small amplitude of an □70-ps decaying component at
     the bluer wavelengths and a rising component of the same duration at the
     redder wavelengths.  The small amplitude component, which comprises no
     more than 20% of the fluorescence decay, is attributed to excited-state
     tautomerization that is mediated by the solvent.  Particular attention
     is paid to the pH dependence of the fluorescence lifetimes and yields.
     Upon tautomerization, the basic 1-nitrogen (N1) of 7-azaindole is
     rapidly protonated giving rise to a species whose emission max. is at □
     440 nm.  The fluorescence emission max. and lifetime of 7-azaindole is
     dominated by the 80% of the solute mols. that are blocked by unfavorable
     solvation from executing excited-state tautomerization.  It is proposed
     that .gtorsim.10 ns is required for the surrounding water mols. to
     attain a configuration about 7-azaindole that is propitious for
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tautomerization.

=> log y
STN INTERNATIONAL LOGOFF AT 10:46:24 ON 29 NOV 2006

=> d his

(FILE 'HOME' ENTERED AT 08:37:41 ON 29 NOV 2006)
FILE 'REGISTRY' ENTERED AT 08:37:51 ON 29 NOV 2006
L1 STRUCTURE UPLOADED
L2 50 S L1
L3 1656 S L1 FULL
FILE 'CA' ENTERED AT 08:39:29 ON 29 NOV 2006
L4 741 S L3
L5 23 S L4 AND FLUORESC?
L6 7 S L5 AND PY<2000
L7 25 S L4 AND PROTON?
L8 22 S L7 AND PY<2000
L9 29 S L6,L8

=> d l9 bib,ab,kwic 1-29

L9 ANSWER 8 OF 29 CA COPYRIGHT 2006 ACS on STN
AN 112:235234 CA
TI Chemistry of benzotriazoles. Benzotriazol-1-ylmethylammonium salts synthesis and reactivity
AU Katritzky, Alan R.; Hughes, Craig V.; Rachwal, Stanislaw
CS Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA
SO Journal of Heterocyclic Chemistry (1989), 26(6), 1579-88
AB Benzotriazol-1-ylmethylamines on treatment with alkylating agents afford benzotriazol-1-ylmethylammonium salts e.g., I (R = Me, Et), also available from reactions of chloromethylbenzotriazole with tertiary amines. In deuterated solvents under basic conditions the methylene protons of these salts exchange with deuterium. At elevated temps., an alkyl group substituent migrated from the ammonium center to the benzotirazolyl N-3. Reaction of the salts with Grignard reagents afforded various products arising from substitution of the ammonium moiety and/or from attack on the benzotriazolyl N-3 or on the benzenoid ring.
IT 13351-73-0P 16584-05-7P 69218-29-7P 127236-93-5P

L9 ANSWER 10 OF 29 CA COPYRIGHT 2006 ACS on STN
AN 111:133584 CA <<LOGINID::20061129>>
TI Tautomerism and aromaticity in 1,2,3-triazoles: the case of benzotriazole
AU Tomas, Francisco; Abboud, Jose Luis M.; Laynez, Jose; Notario, Rafael; Santos, Lucia; Nilsson, Sven Ove; Catalan, Javier; Claramunt, Rosa Maria; Elguero, Jose
CS Fac. Cienc., Univ. Valencia, Valencia, Spain
SO Journal of the American Chemical Society (1989), 111(19), 7348-53
AB This paper provides an explanation for the extraordinary difference in stability between 1,2,3-triazole and benzotriazole tautomers. In the gas phase, the 2H tautomer of 1,2,3-triazole represents more than 99.9% of the equil. mixt.; in benzotriazole the reverse is true (more than

99.99% of 1H tautomer at equil.). To understand the origin of this different behavior, an ab initio study at the 6-31G level was carried out on both tautomers of benzotriazole, on benzotriazolate anion, and on both tautomers of benzotriazolium cation (the 1,2- and the 1,3-H,H+ ions). Theor. results (the proton affinity of 1H-benzotriazole is 10.2 kcal mol-1 larger than that of 2H-benzotriazole) were checked against ICR measurements with excellent agreement (1-methylbenzotriazole is 10.4 kcal mol-1 more basic than 2-methylbenzotriazole). Thermodn. measurements (enthalpies of soln., vaporization, sublimation, and solvation) in three solvents (water, methanol, and DMSO) confirm the predominance of the 1H tautomer in soln. Taking into account lone pair/lone pair repulsions and aromaticity, it is possible to explain the different behavior of 1,2,3-triazole and benzotriazole in the case of neutral mols. and their similarity in the case of protonated species.
IT 13351-73-0, 1-Methylbenzotriazole

L9 ANSWER 15 OF 29 CA COPYRIGHT 2006 ACS on STN
AN 95:50166 CA
TI Kinetics and mechanism of acid and base hydrolysis of cis-chloro (benzotriazole)bis(ethylenediamine)cobalt(III) and cis-chloro(N-methylbenzotriazole)bis(ethylenediamine)cobalt(III) cations
AU Rao, B. Seshagiri; Nanda, Rabindranath; Tripathy, Kumuda Kanta
CS Dep. Chem., Ravenshaw Coll., Cuttack, 753003, India
SO Transition Metal Chemistry (Dordrecht, Netherlands) (1981), 6(2), 97-100
AB The kinetics of acid hydrolysis of Cis-[CoCl(btzH)(en)2]2+ and cis-[CoCl (btzMe)(en)2]2+ complexes (where btzH = benzotriazole, btzMe = N-methylbenzotriazole and en = ethylenediamine) was studied in HClO4 at ionic strength I = 0.25 mol dm-3 at 30-40°. In the 1.0 X 10-1-1.0 X 10-3 mol dm-3 acid strength range, the rate of aquation of the [CoCl(btzH) (en)2]2+ cation follows the relationship: -dln[complex]/dt = k1 + k2KNH [H+]-1, where k and k2 are aquation rate consts. of the acid independent and acid-dependent steps, resp., and KNH is the acid dissocn. const. of the coordinated benzotriazole. cis-[CoCl(btzMe)-(en)2]2+ undergoes acid-independent hydrolysis presumably due to the absence of a labile N-H proton. The base hydrolysis could be followed for the cis-[CoCl (btzMe)(en)2]2+ complex only by measuring hydrolysis rates at 0°.
IT 77968-02-6 (hydrolysis of, kinetics and mechanism of acid and base)

=> log y
STN INTERNATIONAL LOGOFF AT 08:45:09 ON 29 NOV 2006

=> d his

(FILE 'HOME' ENTERED AT 15:33:11 ON 28 NOV 2006)
FILE 'REGISTRY' ENTERED AT 15:33:21 ON 28 NOV 2006
L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 1 S L1-2
L4 17 S L1-2 FULL
FILE 'CA' ENTERED AT 15:36:10 ON 28 NOV 2006
L5 10 S L4

=> d l5 bib,ab,it 1-10

L5 ANSWER 1 OF 10 CA COPYRIGHT 2006 ACS on STN
AN 133:150218 CA
TI Fluorescent indicators for nitric oxide
AU Kojima, Hirotatsu; Nagano, Tetsuo
CS Graduate School of Pharmaceutical Sciences, The University of Tokyo, Tokyo, 113-0033, Japan
SO Advanced Materials (Weinheim, Germany) (2000), 12(10), 763-765
AB Thus the authors have developed novel diamine fluorescent indicators that enable real-time visualization of the prodn. and diffusion of NO in living cells.
IT 287485-98-7

L5 ANSWER 3 OF 10 CA COPYRIGHT 2006 ACS on STN
AN 128:151321 CA
TI Development of a fluorescent indicator for the bioimaging of nitric oxide
AU Kojima, Hirotatsu; Sakurai, Kuniko; Kikuchi, Kazuya; Kawahara, Shigenori; Kirino, Yutaka; Nagoshi, Hiroshi; Hirata, Yasunobu; Akaike, Takaaki; Maeda, Hiroshi; Nagano, Tetsuo
CS Graduate School of Pharmaceutical Sciences, University of Tokyo, Tokyo, 113, Japan
SO Biological & Pharmaceutical Bulletin (1997), 20(12), 1229-1232
AB Nitric oxide (NO) has been reported to play various roles as a signal transmitter. However, detailed functions of NO have yet to be clarified. A fluorescent indicator for NO imaging in living cells was developed. The N-nitrosation of newly designed and synthesized 4-((3-amino-2-naphthyl)aminomethyl)benzoic acid (DAN-1) by NO yielded the highly fluorescent triazole-form. The membrane permeable ester deriv. of DAN-1 (DAN-1 EE) was applied to the imaging of NO produced in activated rat aortic smooth muscle cells. After DAN-1 EE has been loaded into cells, the ester bond is hydrolyzed by intracellular esterase, yielding original DAN-1 with less permeability. The fluorescence intensity of the cells loaded with DAN-1 EE increased according to NO prodn. The imaging method with fluorescent indicators will be significant for the functional clarification of NO in vivo.
IT 202582-08-9P development of a fluorescent indicator for bioimaging of nitric oxide)
(see also same journal 1998, 21, 1247) QP501, B566

L5 ANSWER 10 OF 10 CA COPYRIGHT 2006 ACS on STN
AN 29:28304 CA
OREF 29:3674h-i,3675a-i,3676a
TI Tricyclic compounds in which naphthalene is joined by "ortho fusion" with a heterocyclic compound
AU Fries, K.; Walter, R.; Schilling, K.
SO Ann. (1935), 516, 248-85
AB The heats of combustion of anthracene and phenanthrene were detd. to be 9483.9 ± 1.03 cal./g. and 9457.7 ± 0.84 cal./g., resp.; the heats of evapn. were calcd. to be 12.8 and 12.6 kg. cal. per mole, resp. 2,6-C14H8(OH)2 and Br in dioxane give the 1,5-di-Br deriv., greenish yellow, decompg. 135°; di-Me ether, yellow, m. 280° (decompn.); oxidation with CrO3 in AcOH gives 1,5-dibromo-2,6-dimethoxyanthraquinone, yellow, decompg. 345°; its structure was established by synthesis from 2,3-Br(MeO)C6H3CO2H by heating with P2O5. lin-Naphthotriazole [(2',3',5,4)-

naphtho-(1,2,3-triazole)] (I) gives an Ac deriv., pale yellow, m. 149°; the 1-Me deriv., prepd with alk. Me_2SO_4, m. 175°. Reduction of I with Na-Hg in boiling EtOH gives the 8,9-dihydride (II), m. 157°; N-Me compd., m. 147°; N-Ac compd., m. 173°. Catalytic reduction of I (18 hrs.) gives the 4,5,6,7-tetrahydride (III), m. 162°; N-Ac deriv., m. 114°; N-Me deriv., m. 99°; II is only very slowly further catalytically reduced; angular naphthotriazole (IV) is only very slightly catalytically reduced. I, II or III on oxidation give lin-naphthotriazole-8,9-quinone (V), yellow, m. 242° (decompn.); it does not react with $PhNH_2$ in boiling EtOH; N-Ac deriv., pale yellow, m. 186°; N-Me compd., pale yellow, m. 237°. Reduction of V in Ac_2O gives the tri-Ac deriv. of lin-8,9-dihydroxynaphthotriazole, yellow, m. 165°. I and Cl in AcOH give the 8,9-di-Cl deriv., yellow, m. 291° (decompn.); oxidation gives V. I and Br in AcOH give the 9-Br deriv., bright reddish brown, m. 244° (decompn.); twice as much Br gives the 8,9-di-Br deriv., pale brownish yellow, m. 278° (decompn.); oxidation gives V. I and HCHO in EtOH give the 1-methylol deriv. decompg. 191° with evolution of HCHO and formation of I; it is also decompd. by soln. in dil. NH_4OH or by concd. H_2SO_4. I and $ClCH_2CO_2Na$ in dil. NaOH, refluxed 5 hrs., give the 1-acetic acid deriv., yellow, m. 229°; it is pptd. unchanged from concd. H_2SO_4; heating decomposes it into CO and the 1-Me deriv. of I. I and $ClCH_2COCl$ in boiling C_6H_6 give 90% of the 1-chloroacetyl deriv., greenish yellow, m. 179°; concd. H_2SO_4 gives a citron-yellow soln.; with $AlCl_3$ in $PhNO_2$ there results lin-naphthomorpholone, m. 270°; this also results from condensation of 2,3-$H_2NC_{10}H_6OH$ and $ClCH_2CO_2H$. The heats of combustion of I and IV are 7369.3 ± 0.56 cal./g. and 7349.9 ± 1.02 cal./g., resp. 2,3-$C_{10}H_6(NH_2)_2$ and HCO_2H, refluxed 1 hr., give nearly quant. lin-naphthimidazole (VI), m. 221°; N-Ac deriv., m. 172°; oxidation of VI gives 70% of the 8,9-quinone (VII), yellow or brown-yellow, m. above 400°; NaOH gives an orange-yellow salt; it is repptd. unchanged from concd. H_2SO_4; it does not react with $PhNH_2$ in boiling EtOH; the Me deriv., light yellow, m. 286°; reduction of VII with Zn in Ac_2O gives the tri-Ac deriv. of 8,9-di-hydroxy-lin-naphthimidazole, m. 216°. 2,3-$C_{10}H_6(NH_2)_2$ and AcOH, heated 4 hrs. give the 2-Me deriv. of VI, m. 286°; its 8,9-quinone, yellow, m. above 350°; the Na salt is orange-red; it does not react with $PhNH_2$. The di-Ac deriv. of 1,2-$H_2NC_{10}H_6OH$ with Ac_2O gives the tri-Ac deriv., m. 119.5° (Grandmougin, Ber. 39, 2495 (1906), believed this to be a polymer of the di-Ac deriv.); heating at 240-50° gives 2-methyl-2', 1'-naphthoxazole (VIII), b. 312°; the 1',2'-isomer (IX), b. 302°, m. 41.5°; the 2',3'-isomer (X), b. 310°, m. 87.5°, results from the di-Ac deriv. of 3,2-$H_2NC_{10}H_6OH$, m. 188°, by heating at 258°. The heats of combustion are: VIII 7778.7 ± 1.8 cal./g.; IX 7729.8 ± 6.4 cal./g.; X 7775.8 ± 4.9 cal./g. The following work was undertaken in an effort to prep. 2,3-$C_{10}H_6(NH_2)_2$ by a new method. 2,3-$H_2NC_{10}H_6CO_2H$ (5.6 g.) and 15 cc. AcOH, on refluxing, give 5.5 g. dehydro-2-acetylamino-3-naphthoic acid (XI), m. 173°; heating with AcOH gives the known mono-Ac deriv., which yields XI with Ac_2O. XI and $N_2H_4.H_2O$ in EtOH give 88% of 2-acetylamino-3-naphthoic acid hydrazide (XII), m. 225° (decompn.); the free NH_2 deriv., yellowish green, m. 206-10° (decompn.), results from 2,3-$H_2NC_{10}H_6CO_2Me$ or better from linear benzoisatoic anhydride with $N_2H_4.H_2O$. XII and dil. HCl give 2-acetylamino-2-naphthoic acid azide (XIII), yellow, m. 233° (explosion). Heating XIII in C_6H_6 gives N-acetyl-2,3-naphthoimidazolone, m. 238°; heating XIII in AcOH gives the O-Ac isomer,